A New Technique for Solving Poisson's Equation with High Accuracy on Domains of Any Aspect Ratio

Robert D. Ryne
Lawrence Berkeley National Laboratory

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- J. Qiang, LBNL
- R. Gluckstern, U. Maryland, retired

Critical Issue

- **Poisson solvers used in quasistatic electric and gravitational particle-in-cell simulations generally fail when the grid aspect ratio >> 1**
- **Some important problems involve extreme aspect ratios:**
  - Long beams in rf accelerators: length ~1m; radius ~1mm
  - Beams in induction linacs: length~ 10s of meters; radius ~ cm
  - Galaxies
- **Standard grid-based approaches involve using a very large # of grid points in the long dimension, leading to prohibitively long run times**
- **As a result, it is *extremely* difficult model high aspect ratio systems accurately using standard grid-based approaches**

Observations

- **The Green function, G, and source density, □, may change over vastly different scales**
- **G is known apriori; □ is not**

We should use all the information available regarding G so that the numerical solution is only limited by our approximate knowledge of □

- **Example: 2D Poisson equation in free space**

$$\square(x,y) = \int\int G(x-x', y-y')\square(x',y')dx'dy'$$

Standard Approach (Hockney and Eastwood)

$$\phi_{i,j} = \sum G_{i-i',j-j'} \rho_{i',j'}$$

- **This approach is equivalent to using the trapezoidal rule (modulo treatment of boundary terms) to approximate the convolution integral**
- **This approach makes use of only partial knowledge of G**
- **The error depends on how rapidly the integrand, ϕG, varies over an elemental volume**
  - If ϕ changes slowly we might try to use a large grid spacing; but this can introduce huge errors due to the change in G over a grid length

Cellular Analytic Convolution (CAC)

- Assume the charge density, ρ, varies in a prescribed way in each cell
- Use the analytic form of the Green function to perform the convolution integral exactly in each cell, then sum over cells
- Example: linear basis functions to approximate ρ in a cell:

$$\phi(x_i, y_j) = \sum_{i',j'} \rho_{i,j} \int_0^{h_x} dx' \int_0^{h_x} dy' (h_x - x')(h_y - y') G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\sum_{i',j'} \rho_{i+1,j} \int_0^{h_x} dx' \int_0^{h_x} dy' \, x' (h_y - y') G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\sum_{i',j'} \rho_{i,j+1} \int_0^{h_x} dx' \int_0^{h_x} dy' (h_x - x') y' G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\sum_{i',j'} \rho_{i+1,j+1} \int_0^{h_x} dx' \int_0^{h_x} dy' x' y' G(x_i - x_{i'} - x', y_j - y_{j'} - y')$$

- Shifting the indices results in a single convolution involving an integrated effective Green function:

$$\phi_{i,j} = \sum_{i',j'} G^{eff}_{i-i', j-j'} \rho_{i',j'}$$

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Cost and Accuracy of CAC; Improvement over Standard Approach

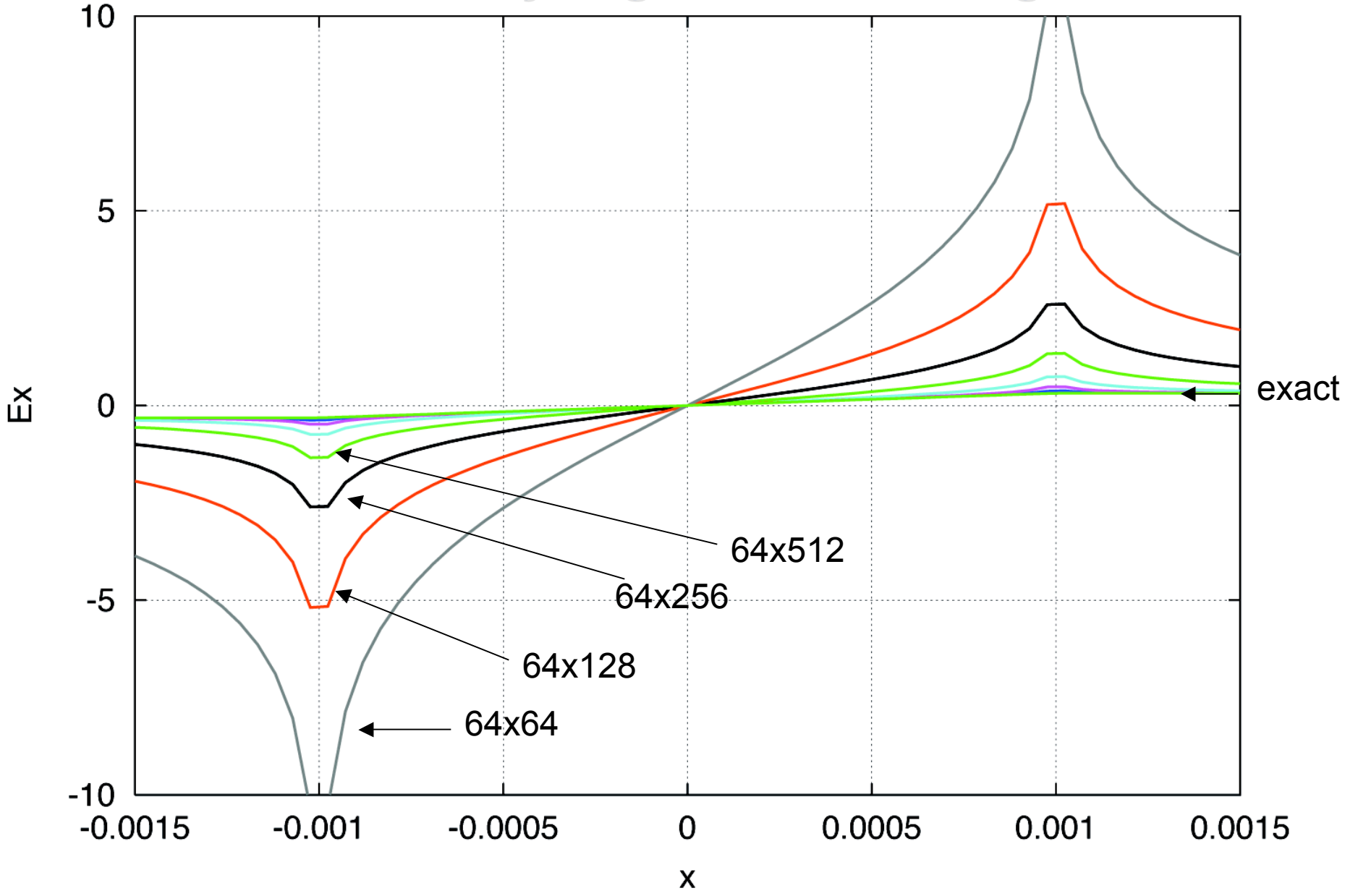
- **Cost: Computing the elemental integrals can be done via analytical formulae in 2D (and 3D?) or by num. quadrature**
  - Requires more FLOPS than simply using G_{ij} but…
  - In situations where the grid is fixed, this only needs to be done once at the start of a run. Amortized over many time steps, this does not significantly impact run time.
- **Accuracy: Method works as long as the elemental integrals are computed accurately and as long as the grid and # of macroparticles are sufficient to resolve variation in □**
- **CAC maintains accuracy even for extreme aspect ratios (>1000:1)**

As a result, CAC performs orders of magnitude better than the standard convolution algorithm for realistic problems involving large aspect ratios

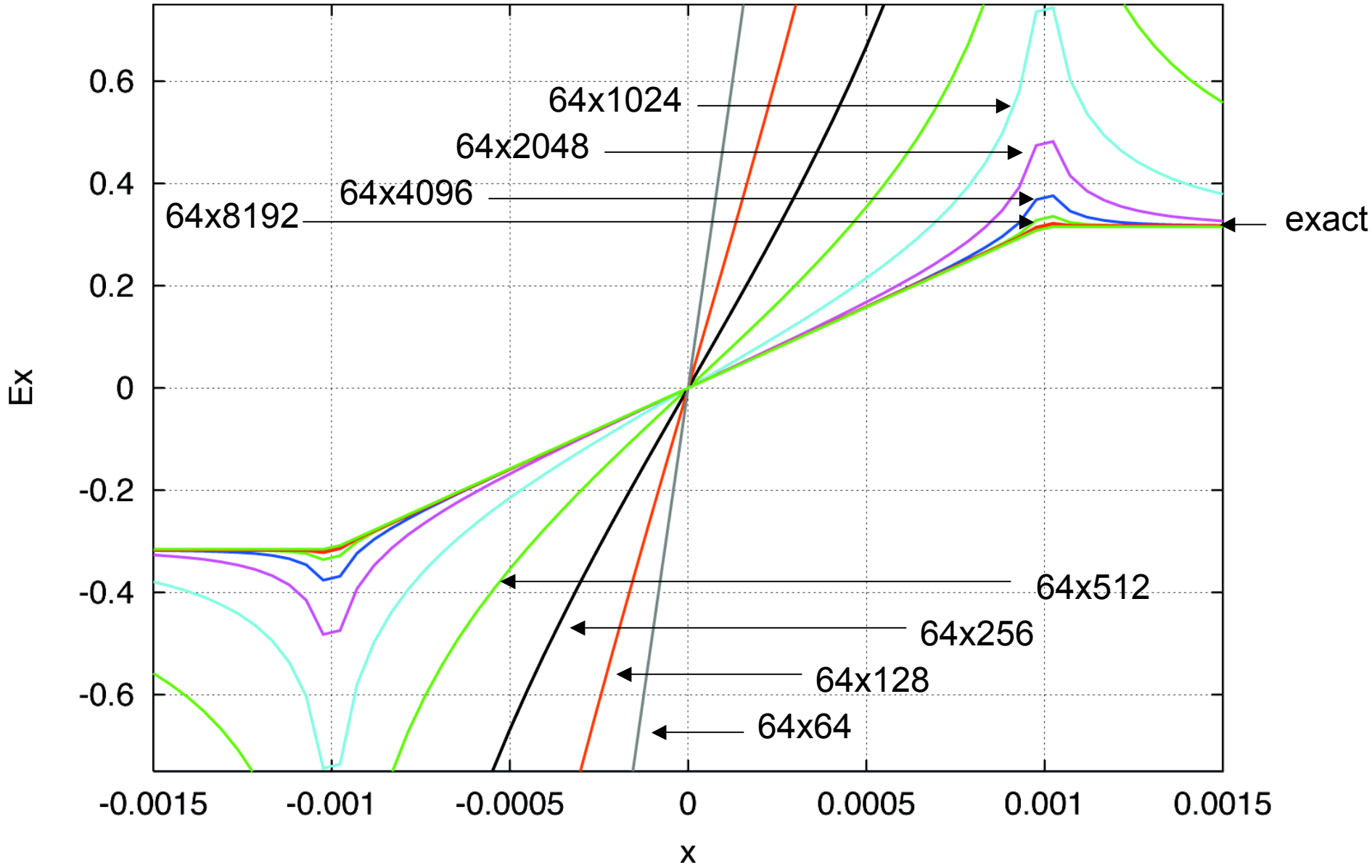
Example: Uniformly filled 2D ellipse

- **Aspect ratio is 1:1000 -- x_{max}=0.001, y_{max}=1**
- **Calculation of fields using (1) standard Hockney algorithm and (2) new CAC approach**
  - In both cases, performed convolutions for the fields directly (rather than calculating the potential and using finite differences to obtain fields)
- **Calculation performed on a grid of size ±0.0015 x ± 1.5 using a mesh of size**
  - Hockney: 64x64, 64x128, 64x256,…, 64x16384
  - CAC: 64x64

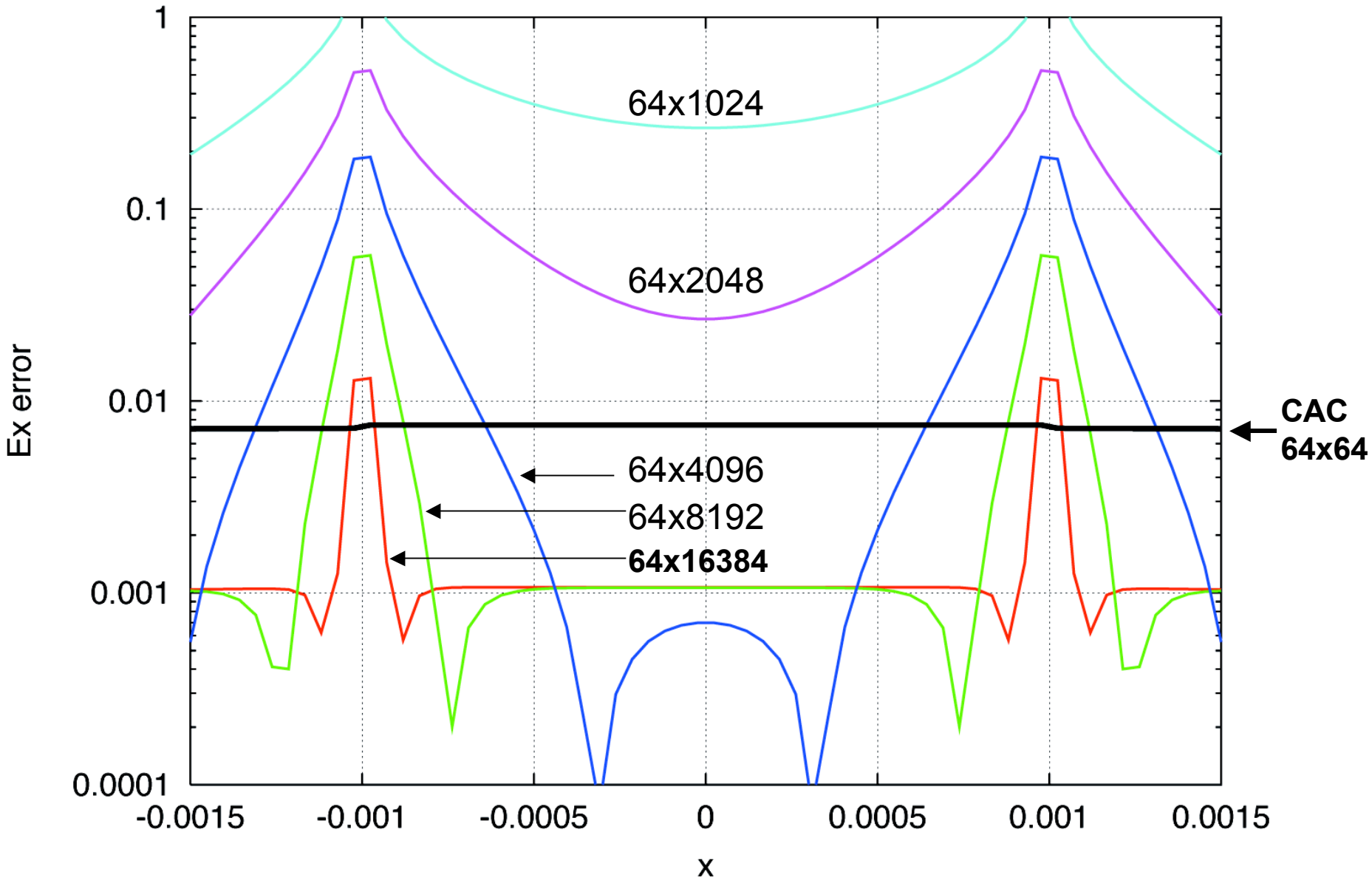
1:1000 test case; Ex vs. x:
Standard Hockney Algorithm has huge errors



Ex vs. x : Reduced Vertical Scale



New algorithm (CAC) provides better than 1% accuracy using 64x64 grid (black curve). Old algorithm is worse everywhere on 64x2048 (purple); error > 10% at some locations on 64x4096 (blue); requires 64x16384 to achieve < 1% everywhere (red).



Bottom Line

- For this test problem, the standard Hockney algorithm would require ~500 times more computational effort to achieve the same worst-case accuracy as a simulation using the new ACE approach.
- CAC works whether the aspect ratio is large, small, or near unity, i.e. it is generally applicable.
- Verified in 2D; we expect the same to hold for 3D

Extension to Beams in Pipes

- CAC provides a crucial advantage, since the Green function falls off exponentially in z, though □(z)may change slowly over meters
- Due to shielding, sum can be truncated in the “long” direction:

$$\square_{i,j} = \sum_{i'=1}^{N_x} \sum_{j'=j}^{j \pm j_{cutoff}} G^{eff}_{i-i',j-j'} \square_{i',j'}$$

- For long beam in a conducting pipe, if grid length in z is >> pipe radius, can truncate at nearest neighbors:

$$\square_{i,j} = \sum_{i'=1}^{N_x} (G^{eff}_{i-i',j-1} \square_{i',j-1} + G^{eff}_{i-i',j} \square_{i',j} + G^{eff}_{i-i',j+1} \square_{i',j+1})$$

- For a rectangular pipe, can rewrite Green function as a sum of convolutions and correlations; then can still use FFT-based approach to sum over elements